

#Ligand	TotalEnerg	VDW	AverConPair
6xs6-Roccustyrna_fr4-0.pdb	406.188	406.188	208.857
6xs6-Roccustyrna_fr6-0.pdb	2079.27	2079.27	416.667
6xs6-Roccustyrna_gs1-0.pdb	-926.867	-926.867	171.667
6xs6-Roccustyrna_gs3-0.pdb	1315.98	1315.98	395.789
6xs6-Roccustyrna_gs4-0.pdb	-103.451	-826.471	136.735
6xs6-Roccustyrna_gs5-0.pdb	-873.398	-873.398	15.275
6xs6-Roccustyrna_gs6-0.pdb	-785.159	-785.159	130.732
6xs6-Acalabrutinib_CID_71226662 (1)-0.pdb	-867.968	-867.968	160.857
6xs6-Ursolic acid-0.pdb	-722.477	-722.477	145.758
6xs6-Valsartan-0.pdb	-795.093	-795.093	165.625